U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Nuclear Energy Advanced Modeling & Simulation (NEAMS) Program Overview

Nuclear Energy University Programs (NEUP) Fiscal Year (FY) 2015 Annual Planning Webinar

Advanced Modeling & Simulation Office (NE-41)
Office of Science and Technology Innovation (NE-4)
U.S. Department of Energy

August 2014

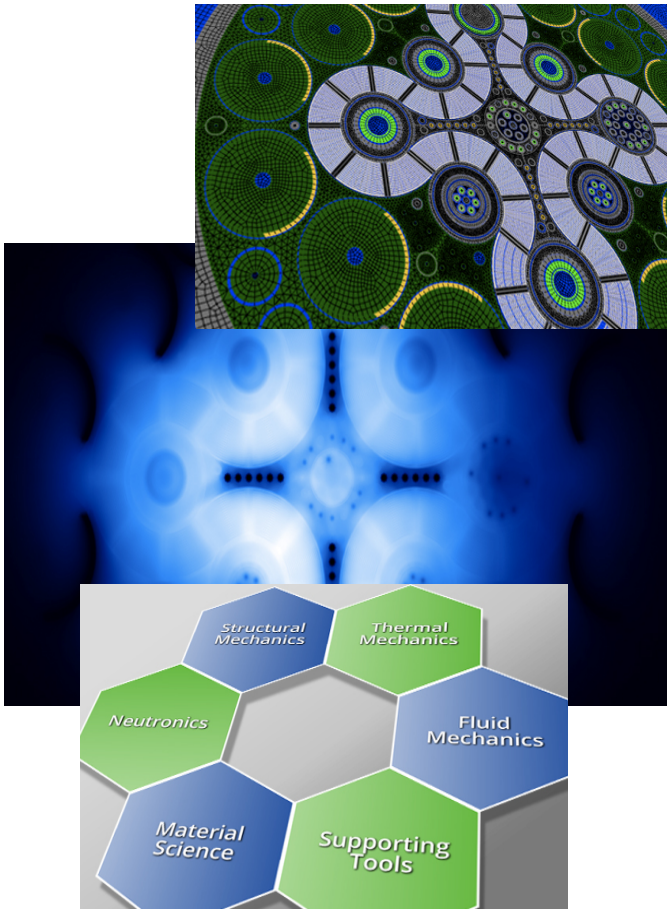
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

Why pursue advanced modeling and simulation capabilities?

- **Modeling & simulation is a critical part of R&D** – *when integrated with theory and experiment, it enhances opportunities for new insights and more effective research*

- **In particular, advanced modeling & simulation offers the ability to gain new insights about the performance and safety of nuclear energy technologies** – *R&D programs are using modeling & simulation; NEAMS is giving them new capabilities for doing so*

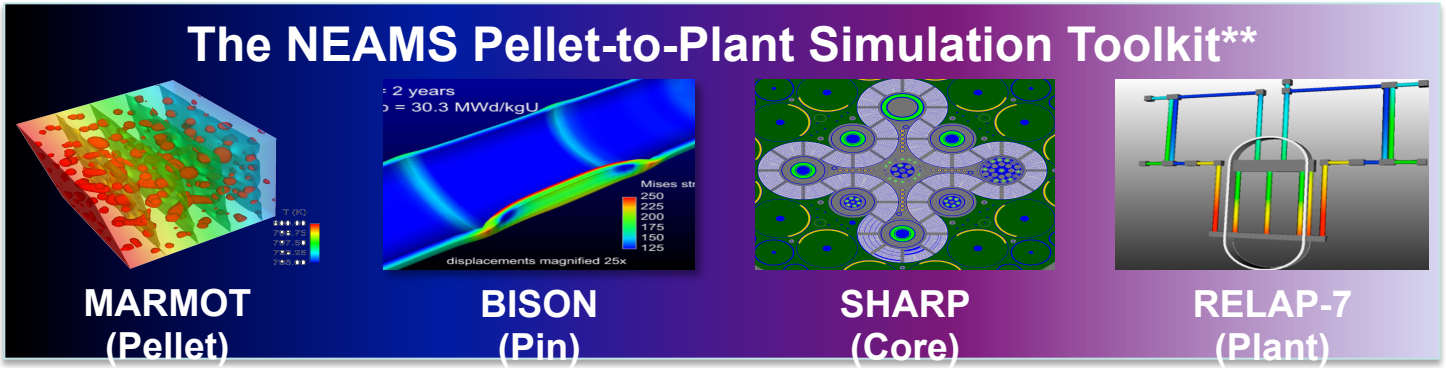


U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

So, what is the Value Proposition for these new capabilities?

- **Mission/Vision:** *These advancements can be deployed as user-friendly simulation toolsets to both the R&D community as well as to industry – will impact existing, near-term and future reactors*
- **Objective:** *Develop and validate predictive analytic computer methods for the analysis and design of reactor and fuel cycle systems, and demonstrate the impact and potential of these new capabilities by collaboratively solving stakeholder-defined high-impact problems*
- **Value Proposition:** *Produce a NEAMS Pellet-to-Plant ToolKit that will*
  - *provide insights and problem solutions that cannot be achieved through experimentation alone*
  - *have the potential to enhance the development and implementation of new reactor and fuel cycle concepts*

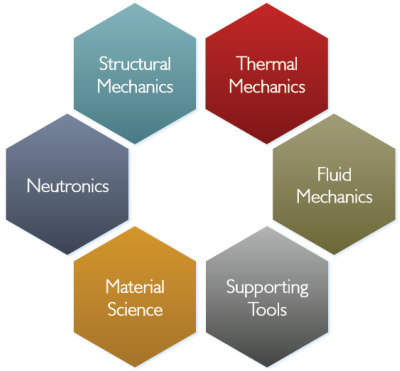


U.S. DEPARTMENT OF ENERGY
Nuclear Energy

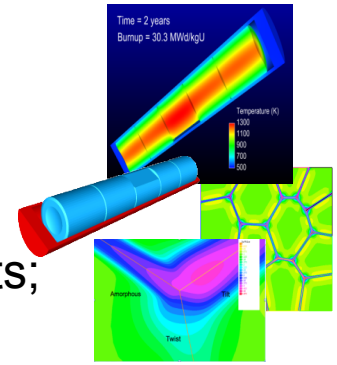
Nuclear Energy Advanced Modeling and Simulation (NEAMS)

So, how do we do all this? NEAMS is organized into two Product Lines –

- **Fuels Product Line:** Supports advanced fuels development.

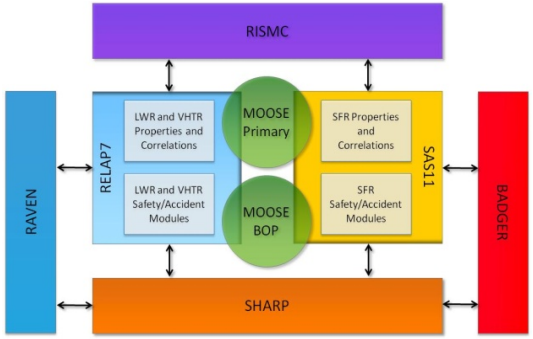


- **Reactors Product Line:** Supports advanced reactors development.
- **Both Product Lines:** Support validation efforts; solving high-impact problems; RELAP-7



But the key is the NEAMS Team –

- **Multi-lab, Multi-discipline, and dedicated:**
  Participants from over seven labs across the DOE complex

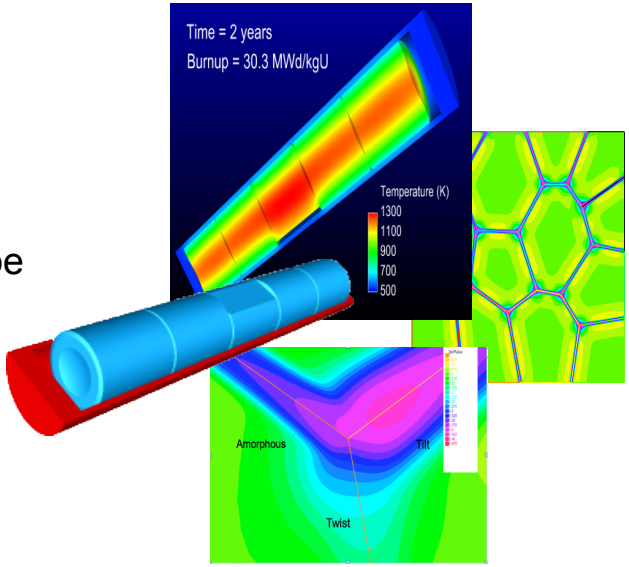


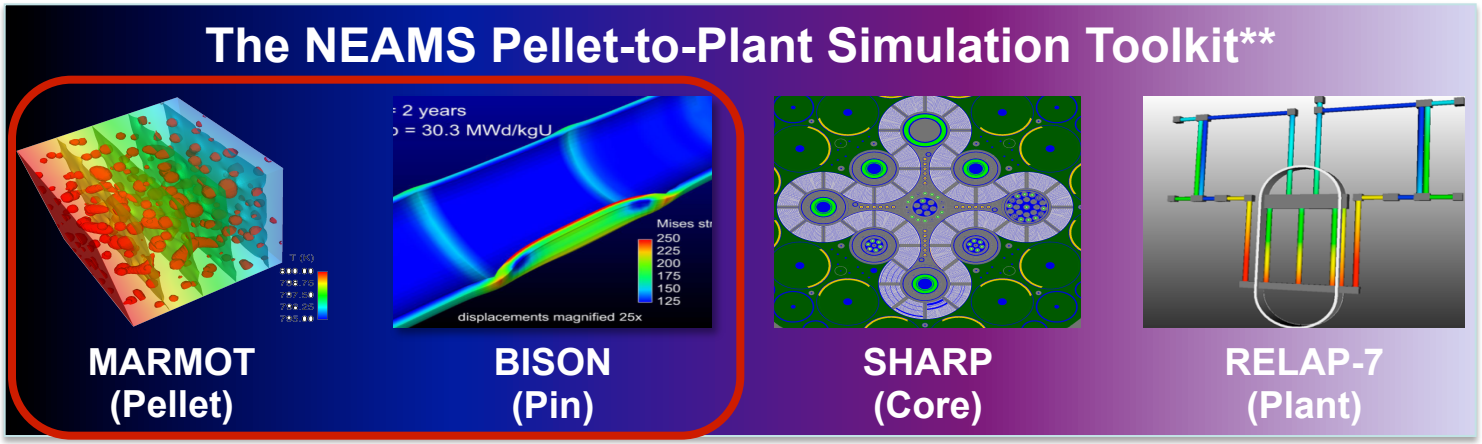
- **Leadership Council:**
  - NEAMS National Technical Director, **Dr. Marius Stan**, DOE;
  - Fuels Technical Lead, **Dr. Steven Hayes**, INL;
  - Reactor Technical Lead, **Dr. Keith Bradley**, ANL;
  - Integration Lead, **Dr. Dave Pointer**, ORNL (*Dave is also the NEAMS Lab TPOC for NEUP*)

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Fuels Product Line*

- **The FPL spans "pellet to pin" fuel simulation**
- **Goal is to be able to apply the FPL Toolset (in the NEAMS Toolkit) to several Fuels R&D areas**
  - Advanced fuel designs; Accident-tolerant fuels research; could be extended to simulate behavior of used fuel in long term storage
- **Focus is to develop mechanistic (truly predictive) computational capabilities for multi-scale fuel performance simulation (stand-alone or coupled)**

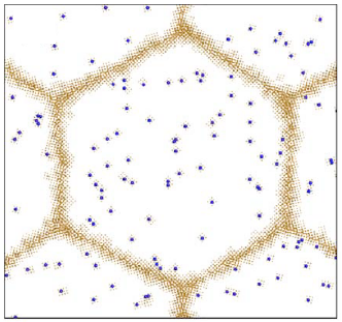




NEAMS – *Fuels Product Line*

- **So, the if goal is to develop true predictive capability then we need to use a multi-scale modeling approach**
  - Empirical models can accurately interpolate between data but cannot accurately extrapolate outside of test bounds
  - Thus our goal is to develop improved, *mechanistic materials models* for fuel performance using hierarchical multiscale modeling

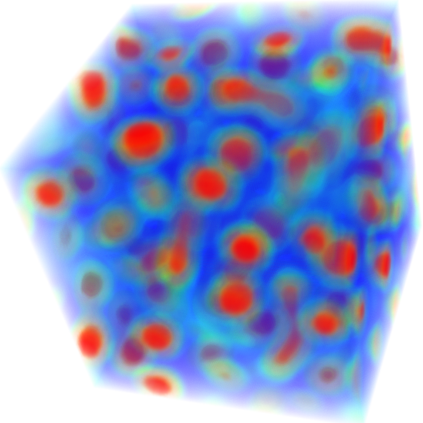
Atomistic simulations



- Identify important mechanisms
- Determine material parameter values

Atomistically-informed parameters

Meso-scale models

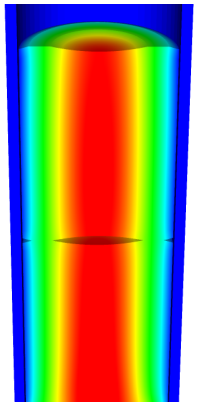


- Predict microstructure evolution
- Determine effect of evolution on material properties

Degrees of freedom, operating conditions

Meso-scale informed materials models

Fuel performance models

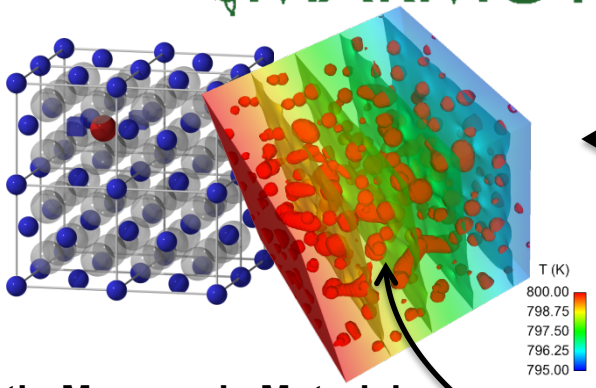


- Predict fuel performance and failure probability

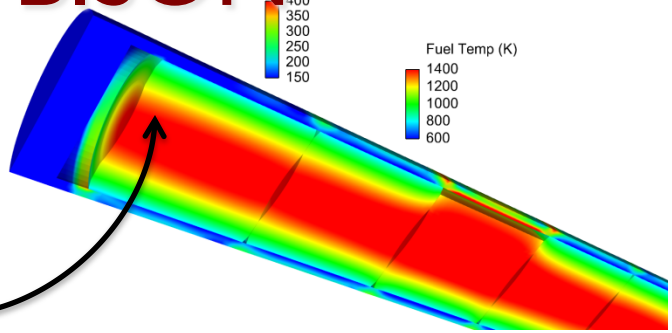
NEAMS – *Fuels Product Line*

- **FPL Toolset: MOOSE-BISON-MARMOT (advanced, multiscale fuel performance capability)**

MARMOT



BISON



Atomistic-Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations
- **BISON Theory, Users, & Assessment Manuals (plus other good info) can be found at: http://www.inl.gov/BISON**

NEAMS – *Fuels Product Line Activities*

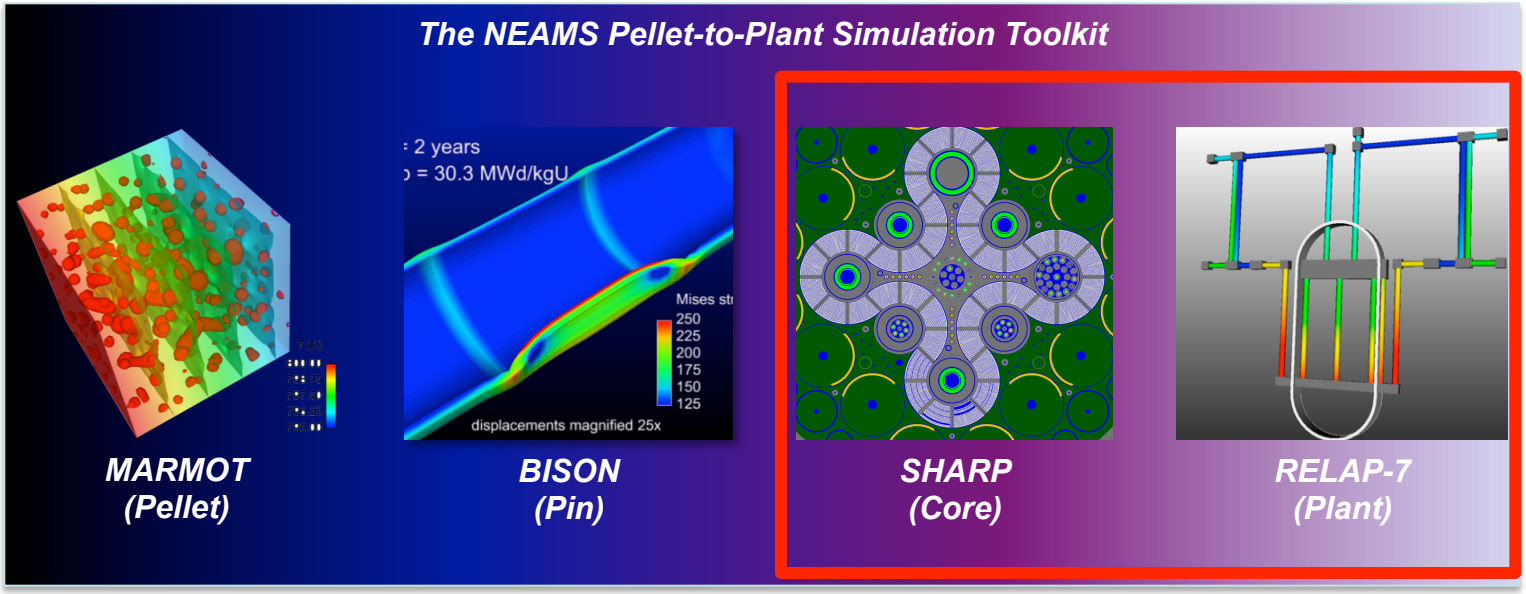
- **Current focus is primarily on developing BISON as the engineering-scale fuel performance tool for simulating oxide fuel pins. Ongoing work will improve/enhance BISON in several key ways:**
  - **More robust mechanical contact and solid swelling models**
  - **Extension of smeared cracking model to 3D, coupled to fuel creep models**
  - **Cladding creep models coupled to plasticity for rapid power transients.**
  - **Implementation of stress-based fuel densification model.**
  - **Enhanced coolant sub-channel model for LOCA (*i.e., boiling curve, DNB, reflood/quench*)**
  - **Validation and assessment studies (*against selected, relevant pins from the FUMEX-II,III, ENIGMA, and Halden LOCA databases*).**

- **Additional/future work includes:**
  - **Investigating coupling of multiple material models and development of the contact algorithm (*to increase code robustness*)**
  - **Spent Fuel Demonstration (*preliminary "cradle to grave" capability*)**
  - **Halden 3D Experiment Planning - groundwork for an experiment to be performed by the OECD Halden Reactor Project.**

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactors Product Line*

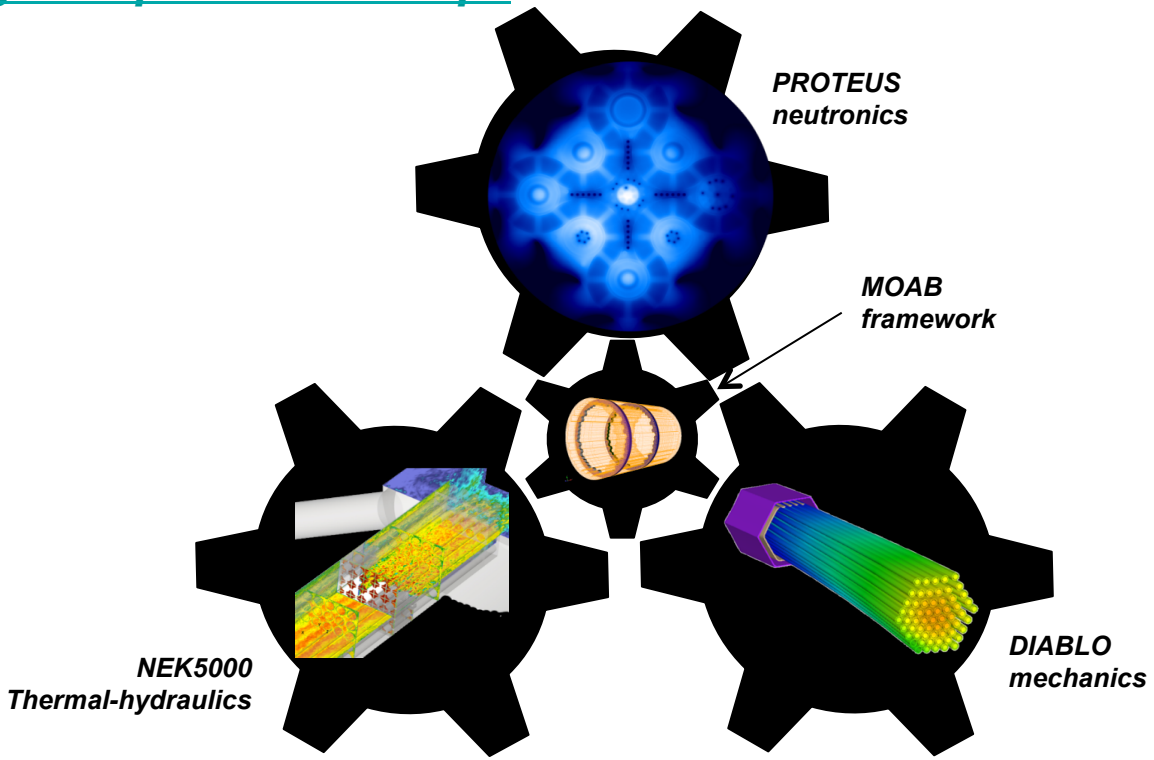
- The RPL spans the reactor "core to the full plant"



- AIM: a "seamless interoperability option"
- CURRENT EMPHASIS: robust, useful stand-alone products
- FUTURE PROOF: This enables traditional workflow but positions the toolkit for future approaches and superior predictability where needed

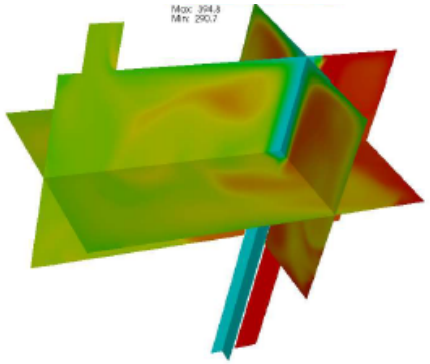
NEAMS – *Reactor Product Line*

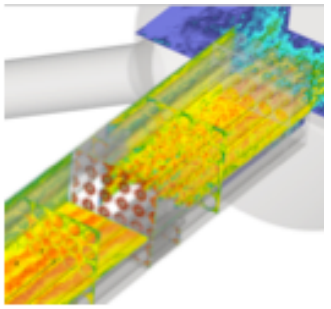
- **SHARP – central to the "interoperability" approach**
  - *Intrinsically Multi-Physics and Multi-Scale*
  - *Coupling when necessary*
  - *Stand-alone when sufficient*
  - ***http://www.ne.anl.gov/capabilities/sharp/***

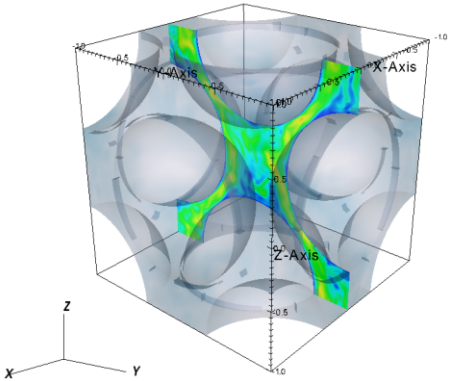


NEAMS – *Reactor Product Line*

Nek5000 – the NEAMS Reactor Thermal Fluids Module



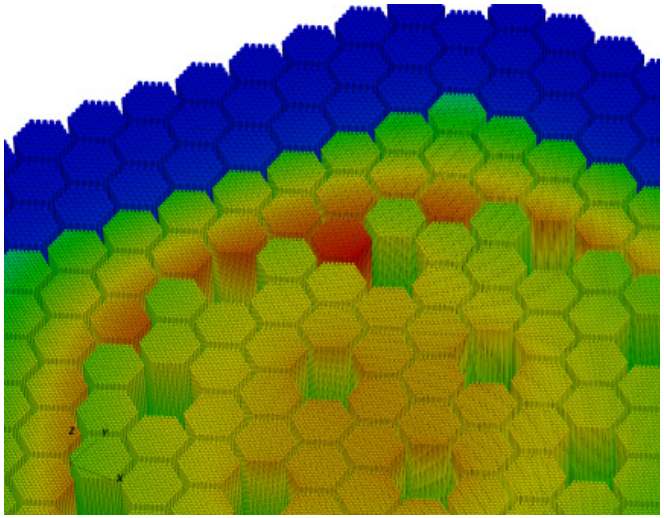


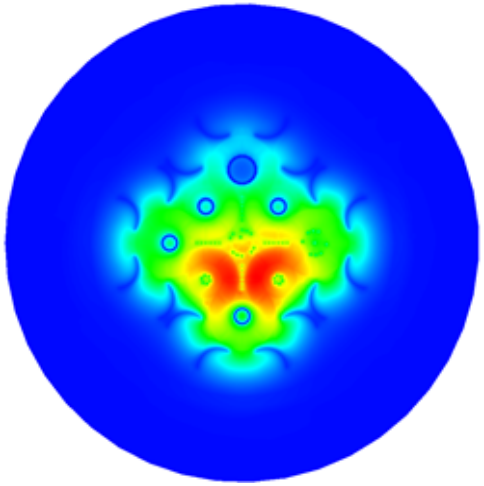


- **Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics**
  - Computational Fluid Dynamics (CFD) toolset using the Spectral Element Method (SEM)
    - Accurate high order solutions (Order 4-16)
    - Provides excellent convergence and solution verification characteristics
  - High fidelity solutions using Direct Numerical Simulation (DNS) and a variety of Large Eddy Simulation (LES) methods
  - Intermediate fidelity solutions using Unsteady Reynolds Averaged Navier Stokes (URANS) methods
  - Reduced fidelity modeling using porous media approaches.
  - Supports conjugate heat transfer analysis
  - Includes Stability Analysis toolkit with adjoint and Proper Orthogonal Decomposition capabilities
- **Open Source – available for download at nek5000.mcs.anl.gov**
- **Validation in progress for many nuclear energy applications**
  - T-junctions, spacer grids, wire-wrapped fuel assemblies, jet/plenum mixing
  - More needed
- **Demonstrated for up to 1,000,000 cpu processes and several billion geometric grid points.**
  - Also runs on desktop workstations

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line*

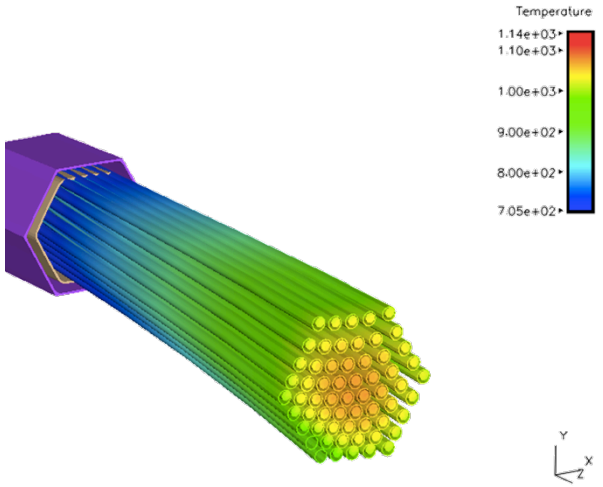


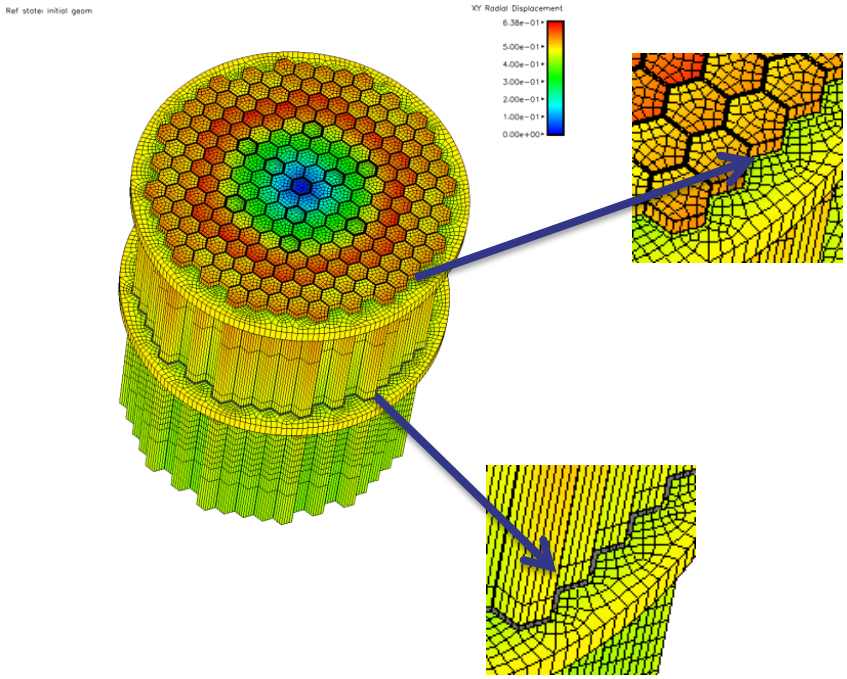


- **The SHARP neutronics module, PROTEUS**
  - Neutral particle transport solvers including 2nd order S_n method
  - Includes a variety of pre-conditioning options
  - Supports pseudo-state and adiabatic
  - Cross-section processing tools
    - *Ultra-fine group structure cross-section library generation (MC-2)*
    - *Sub-group method API and libraries*
- **http://www.ne.anl.gov/pdfs/PROTEUSbrochure_v6.pdf**
- **Early user releases available, with user guides, methodology manuals, etc. in development**
- **Successfully used on real problems- ATR, ZPR, MONJU, PHENIX, EBRII…**
- **Validated against ZPR experiment foil reaction rates and k-effective**
  - More needed!
- **Demonstrated scalability to more than 200,000 CPU cores and billions of degrees of freedom.**
  - Also runs on desktop workstations

NEAMS – *Reactor Product Line*

- **The SHARP Structural Mechanics module, DIABLO**
  - 3-D thermal-structural and thermal mechanics analysis using a time explicit Finite Element Method (FEM)
  - prediction of deformation and stresses under structural and thermal loads
  - Includes a variety of contact modeling options
  - Includes connectivity to selected soil-structure interaction models for seismic analysis

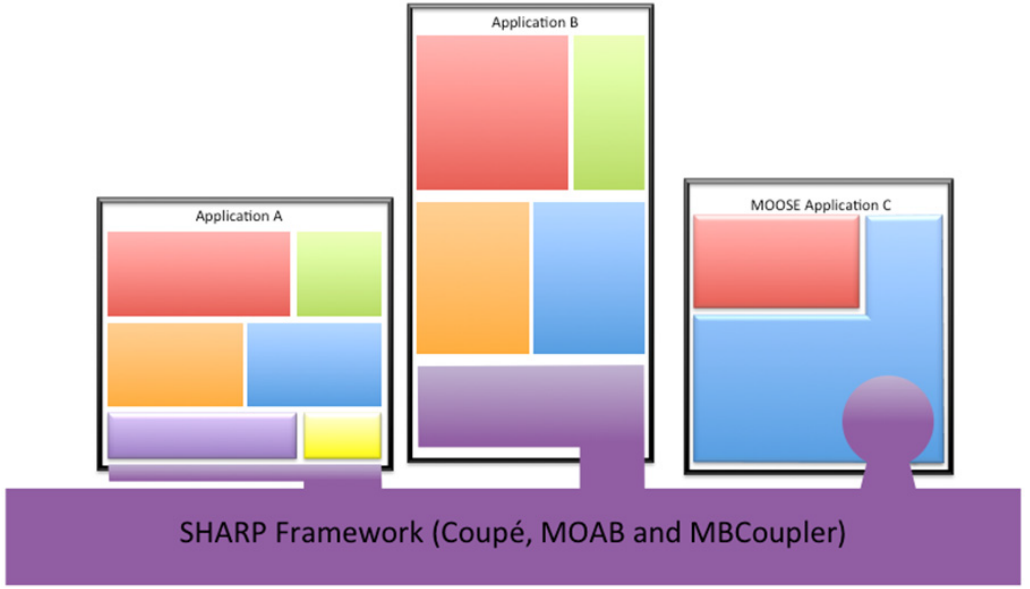




- **Early user releases available, with updated user guides, methodology manuals, etc. in development**
- **Validated for a variety of standard structural mechanics benchmark**
  - Additional specific nuclear energy application validation needed
- **Demonstrated scalability to petascale computing platforms and large problems**
  - Also runs on desktop workstations

NEAMS – *Reactor Product Line*

- **The SHARP framework, illustrated conceptually here, provides a library of tools for integrating different applications to form a single interconnected model**
  - The **Coupé** driver launches the applications integrated by the SHARP framework and monitors their progress to determine when data should be exchanged between modules
  - The **MOAB** code library provides utilities for management of mesh-based data and associated meta-data
  - The **Coupler** library provides tools to support the transfer of data from the computational mesh used by one application to the computational mesh used by another application
  - MOAB and MeshKit are now part of a larger DOE-SC project called SIGMA - **http://press3.mcs.anl.gov/sigma**



- **SHARP Framework applications**
  - Application A – MOAB used as an external companion, where it receives information from the existing data management components of the application
  - Application B – MOAB used as the native data management component for an application
  - Application C – Connectivity (under development) between the MOOSE and SHARP frameworks, creating opportunities for the development of hybrid operator schemes

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **For Program Support in Science & Technology Innovation – NEAMS-1**
  - Seeking proposals that contribute to improving the **mechanistic models**, **computational methods**, and **validation** of NEAMS tools in the toolkit [MARMOT, BISON, SHARP, RELAP-7]
- **Proposals may include:**
  - New models of materials properties as function of reactor environment parameters such as temperature or neutron flux
  - New mathematical or computational methods for improving scale or physics coupling
  - New experimentation designed explicitly for validation, analysis of existing benchmark datasets, development of new benchmark datasets, calibration of models, as well as direct comparison of datasets with toolkit simulations
- **Model development and validation can span the entire hierarchy from single-scale and single-effects experiments designed to address individual phenomena to integrated models or experiments that address strong coupling of multiple phenomena**
- **Running simulations or conducting experiments at DOE laboratories in support of the NEAMS Toolkit are encouraged, although computation or experimentation at university laboratories is equally acceptable. Collaboration with members of the NEAMS development team residing at DOE laboratories is strongly encouraged.**

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – NEUP *Workscope Description*

- **Known priorities include ideas that**
  - Accelerate work to extend of the NEAMS ToolKit's Fuels Product Line's macroscale (Bison) and mesoscale (Marmot) components to fuel types other than conventional LWR oxide fuels
  - Expand the applicability of the NEAMS neutronics module (PROTEUS) to a wider range of transients and demonstrate it's applicability to a wider range of reactor core configurations,
  - Expand the turbulence modeling options available in the NEAMS thermal fluids module (Nek5000) and demonstrate it's applicability to a wider range of reactor types and conditions, and
  - Expand the validation of the NEAMS structural mechanics module (Diablo) and implement models within it which enhance it's ability to predict the behavior of reactor structures, possibly leveraging the ToolKit's existing meso-scale capabilities.
- **POCs**
  - Federal – Dan Funk (dan.funk@hq.doe.gov; 301-903-3845)
  - Technical – Dave Pointer (pointerwd@ornl.gov; 865-241-4472)

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Nuclear Energy Advanced Modeling & Simulation (NEAMS) Program Overview

Nuclear Energy University Programs (NEUP) Fiscal Year (FY) 2015 Annual Planning Webinar

Advanced Modeling & Simulation Office (NE-41)
Office of Science and Technology Innovation (NE-4)
U.S. Department of Energy

August 2014

Back-up Slides

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

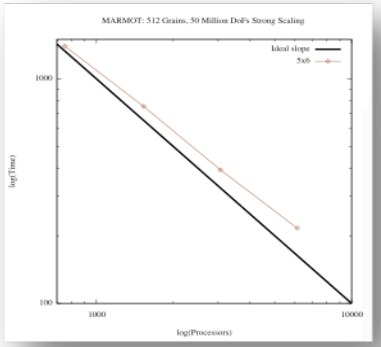
NEAMS – *Fuels Product Line*

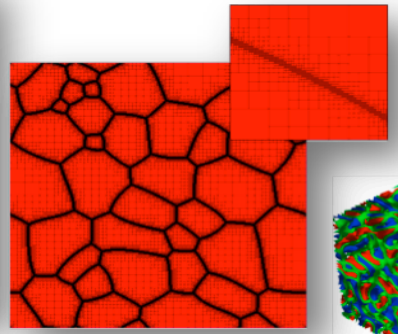
- **MARMOT predicts the coevolution of microstructure and properties due to applied load, temperature gradients and radiation damage**

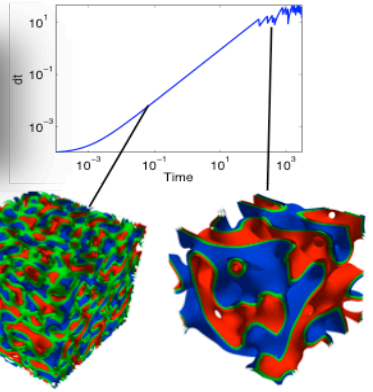
Technique: Phase field coupled with large deformation solid mechanics and heat conduction solved with implicit finite elements using the **MOOSE** framework

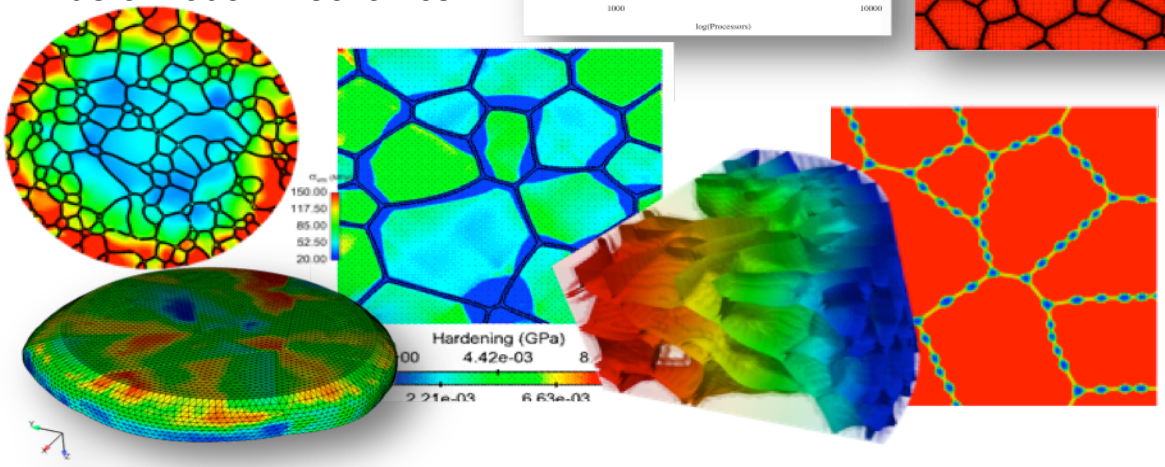
Numerical capabilities:

- Massively parallel, from 1 to 1000's of processors
- Mesh adaptivity
- Time step adaptivity
- Small and finite deformation mechanics









Physical models

- Grain growth/GB migration
- Bubble growth and migration
- Species redistribution
- Stress effects on evolution
- Crystal plasticity

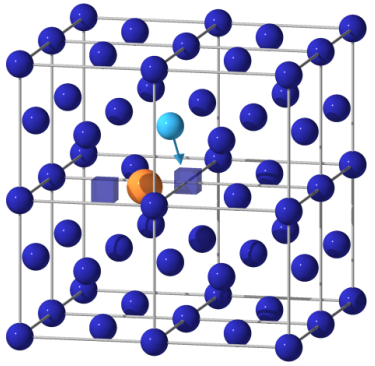
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Fuels Product Line*

- **Example: Various methods are employed at different scales to investigate the different stages of Fission Gas (FG) release:**
  0. Diffusion of individual FG atoms in bulk UO_2+nucleation growth and resolution of intergranular bubbles.
  1. Xe segregation, clustering and bubble nucleation
  2. Bubble growth and coalescence
  3. Percolation in polycrystalline networks

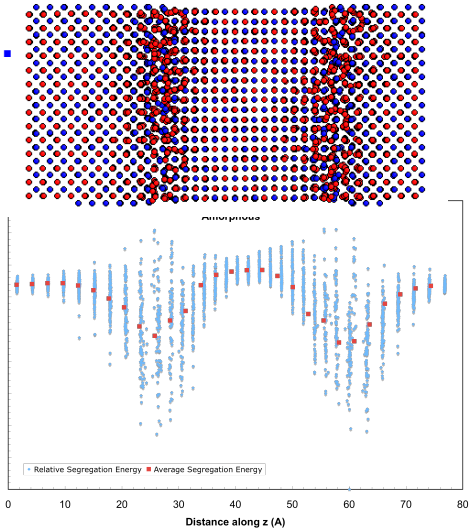
DFT and molecular dynamics

0.



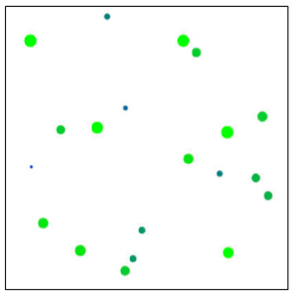
Molecular dynamics

1.



Kinetic Monte Carlo

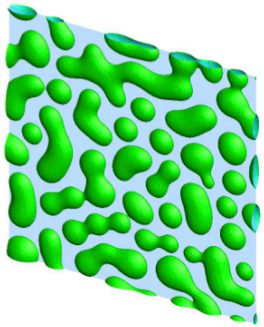
1.



Xe clustering vs. UO_2 boundary type

Phase Field Modeling

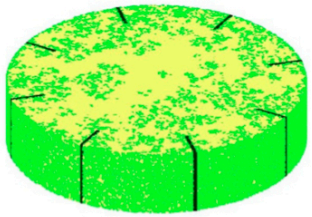
2.



Bubble growth and coalescence

Percolation Analysis

3.



Percolation in polycrystalline networks

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Fuels Product Line*

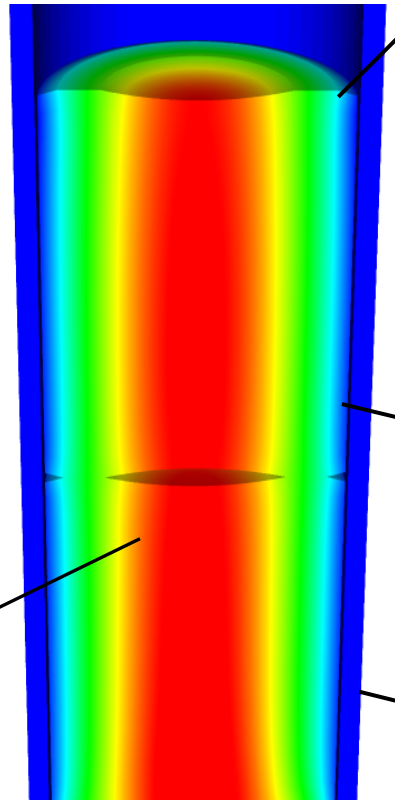
Current BISON capabilities –

General Capabilities

- Finite element based 2D-RZ and 3D fully-coupled thermo-mechanics with species diffusion
- Linear or quadratic elements with large deformation mechanics
- Steady and transient operation
- Massively parallel computation
- **Meso-scale informed material models**
- Applicable to LWR, TRISO, and metallic fuels

Oxide Fuel Behavior

- **Temperature/burnup dependent conductivity**
- Heat generation with radial and axial profiles
- Thermal expansion
- Solid and gaseous fission product swelling
- **Densification**
- **Thermal and irradiation creep**
- **Fracture via relocation or smeared cracking**
- **Fission gas release** (2-stage Forsberg-Massih)



Temperature

Gap/Plenum Behavior

- Gap heat transfer with $k_g = f(T, n)$
- Mechanical contact (master/slave)
- Plenum pressure as a function of:
  - evolving gas volume (from mechanics)
  - gas mixture (from FGR model)
  - gas temperature approximation

Cladding Behavior

- Thermal expansion
- **Thermal and irradiation creep**
- Irradiation growth
- Gamma heating
- **Combined creep and plasticity**

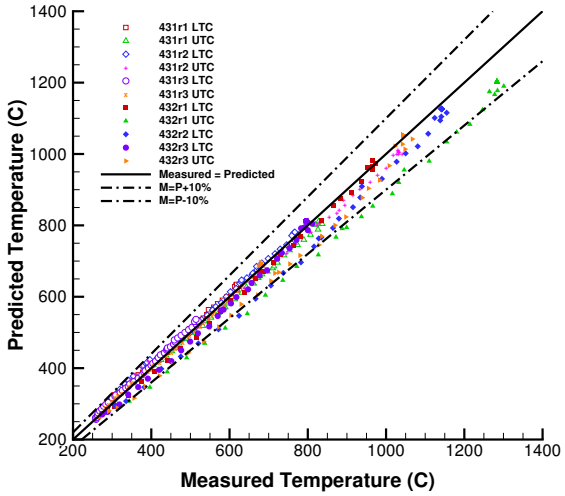
Coolant Channel

- Closed channel thermal hydraulics with heat transfer coefficients

Legend:
Subject of lower-length scale model development

NEAMS – *Fuels Product Line Validation*

- **To date, focus of BISON validation activities have been *primarily* on:**
  - Experimental data sets (88 pins) used for Assessment and Validation of FRAPCON (**not** a comparison with FRAPCON code predictions, but with the experimental data used to validate the FRAPCON code)
  - Includes instrumented fuel pins with steady-state and ramp data relevant to:
    1) Fuel centerline temperature
    2) Fuel restructuring
    3) Gap conductance
    4) Fission gas release
    5) Pellet-cladding mechanical interaction
    6) Cladding elongation
  - Value in assessment against well-known, well-accepted (by NRC) experimental data



Experiment	Rod	FCT - BOL	FCT – TL	FCT - Ramps	FGR	Clad - Elong	Clad – Dia (PCMI)
IFA-431	1, 2, 3	X					
IFA-432	1, 2, 3	X					
IFA-513*	1, 6	X	X				
IFA-515.10	A1	X	X				
IFA-597.3	7			X		X	
IFA-597.3*	8			X			
RISO-3*	AN3			X	X		
RISO-3*	AN4			X	X		
FUMEX-II	27(1)				X		
FUMEX-II	27(2a)				X		
FUMEX-II	27(2b)				X		
FUMEX-II	27(2c)				X		
RISO-3	GE7						X
OSIRIS	J12						X
REGATE							X
IFA-431 (3D)	4	X					

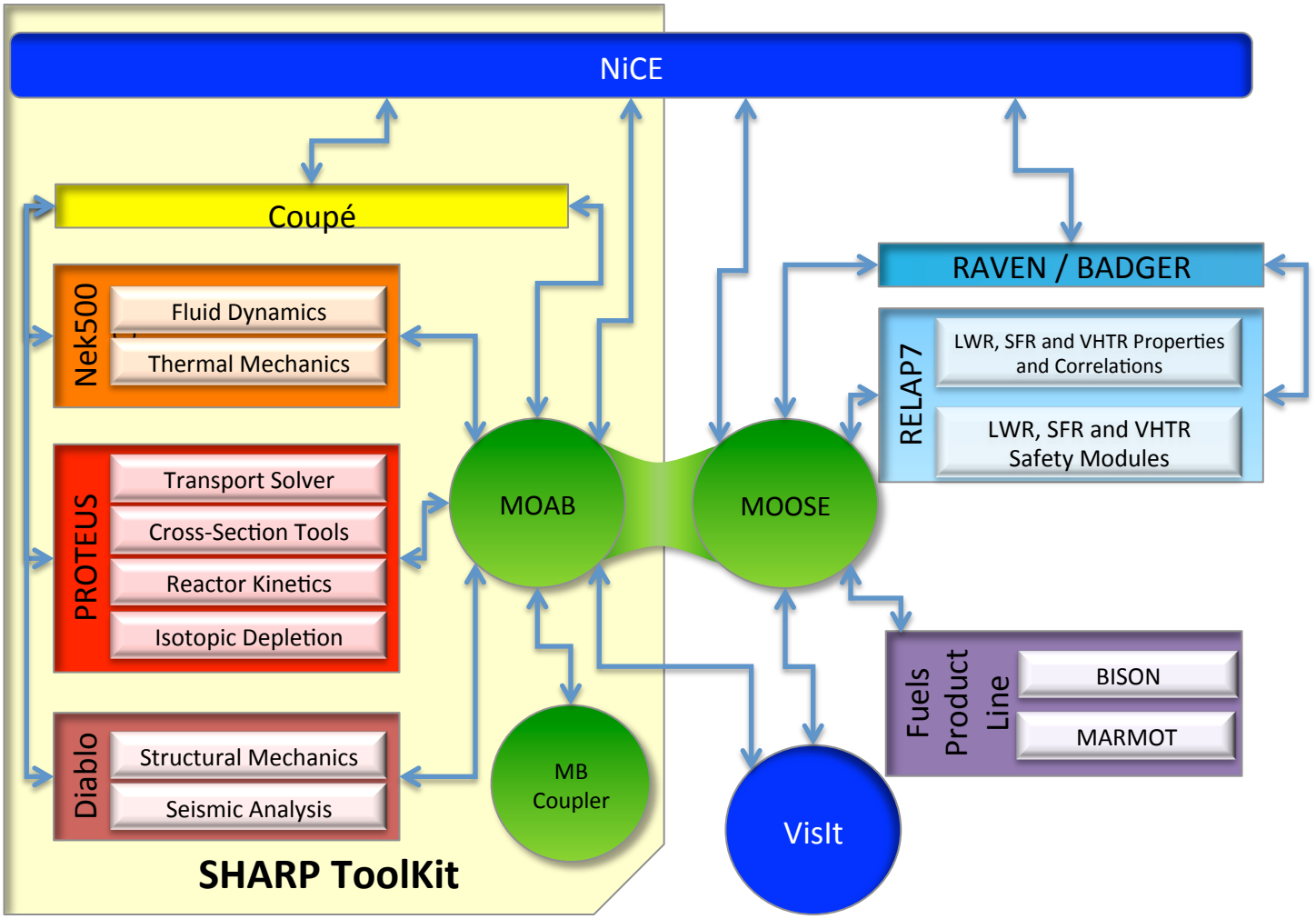
* "Early User" assessment problems

NEAMS – *Fuels Product Line Users*

- **BISON is being used by multiple NE R&D Programs: 6 DOE laboratories, 4 universities, Anatech, and the National Nuclear Laboratory in the UK**
  - ☑ **NEAMS:** The Fuels Product Line leads the development of BISON for simulating the performance of advanced fuel forms for many applications.
  - ☑ **CASL:** MPO is using Peregrine, a version of BISON with selected (proprietary) performance models from EPRI for analyzing fuels challenge problems.
  - ☑ **FCRD:** The Advanced Fuels Campaign is using BISON to model/analyze advanced oxide and metallic transmutation fuel experiments in the ATR as well as Accident Tolerant Fuels concepts currently under development.
  - ☑ **LWRS:** The Advanced LWR Fuels R&D Pathway is incorporating models into BISON to analyze LWR fuel performance with SiC cladding.
  - ☑ **NGNP:** Used for special investigations of asymmetrical fuel particles, defects in coating layers, and failure thresholds during accident scenarios.
  - ☑ **RERTR:** The fuel development program is incorporating models into BISON to analyze low-enriched, high-density U-Mo fuel plate performance.

NEAMS – *Reactor Product Line*

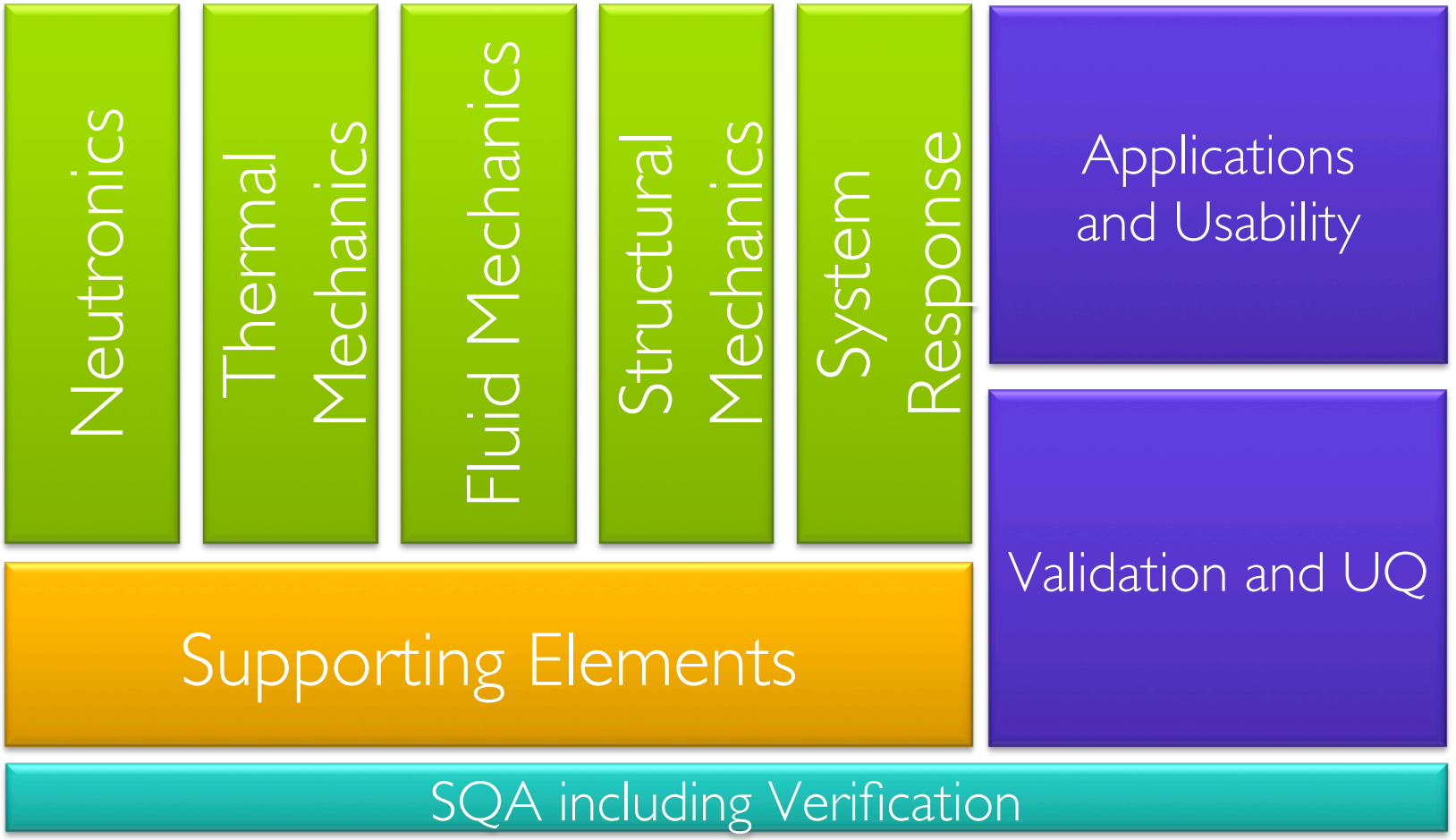
RPL Toolkit component map –



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line*

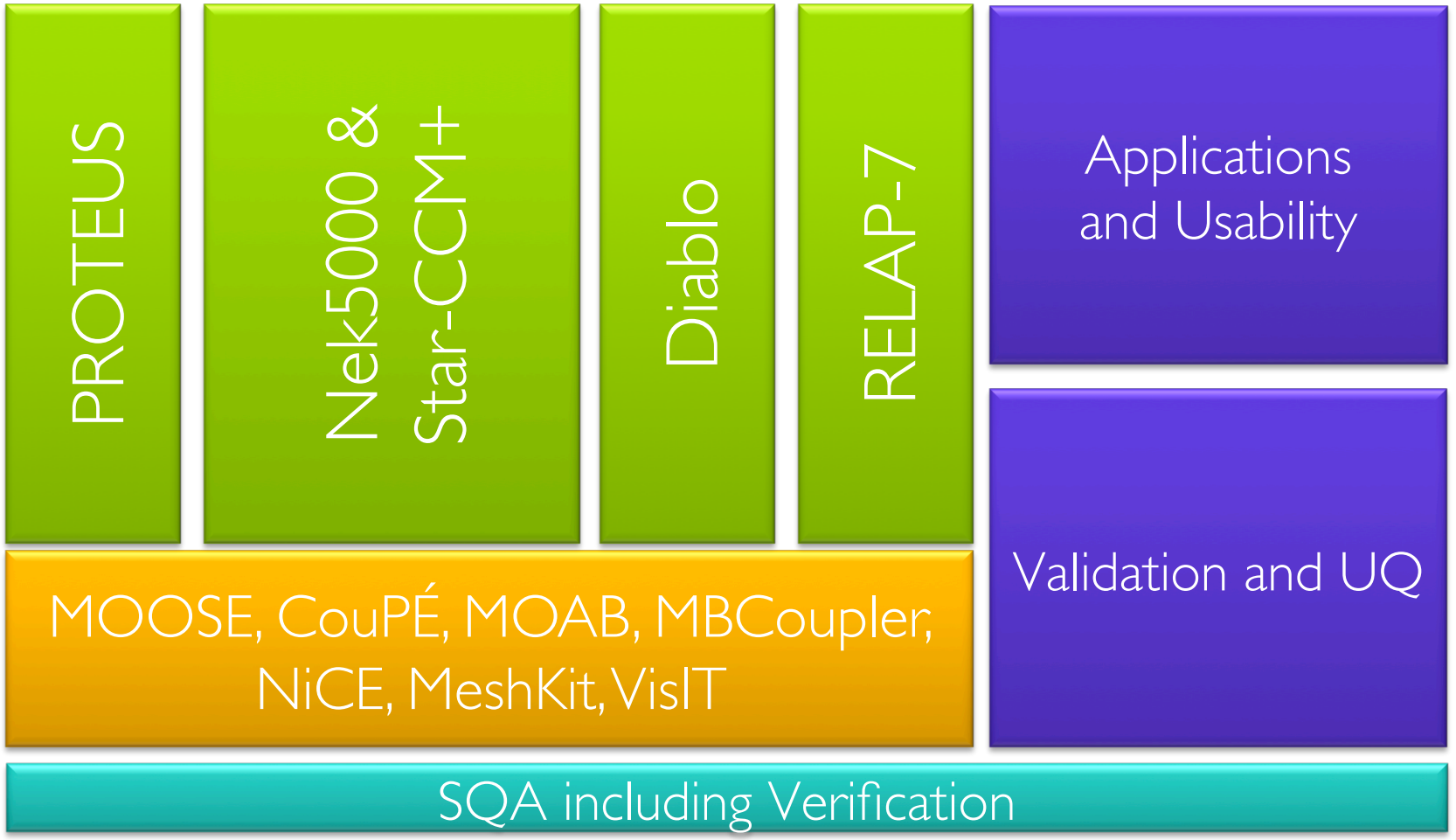
Multi-physics/multi-scale development roadmap –



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line*

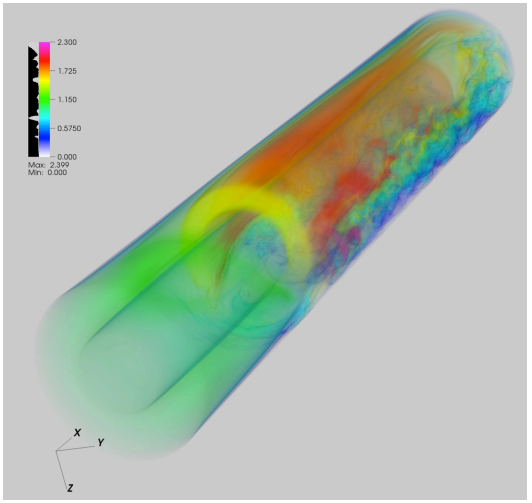
Multi-physics/multi-scale development roadmap –



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS – *Reactor Product Line Validation*

- **NEAMS will provide baseline validation for every physics module**
  - Left to end user to execute application specific validation based on their own PIRT, GDCs and FOM
- **Have established validation plans for every physics module**
  - Neutronics – Build on DIFF3-D/Variant validation database
  - Structural Mechanics – Build on NIKE3D validation database
  - Thermal Fluids – Custom validation plan
    - New DOE Data – MAX, NSTF, MIR
    - New NEUP Data
    - International Collaborations
      - Russian Federation Collaboration (IBRAE, IPPE)
      - Euratom I-NERI
      - KAERI I-NERI
  - RELAP-7
    - Custom validation plan based on EPRI collaboration



- **Will validate integrated RPL toolkit using EBR-II SHRT data**
- **Working to establish validation pathway for new data**

U.S. DEPARTMENT OF ENERGY

Nuclear Energy

NEAMS – *Reactor Product Line Users*

- RELAP-7 reactor safety
- Diablo structural mechanics
- PROTEUS neutron transport
- MC^2-3 ultra fine cross sections
- NiCE user environment
- MOAB data backplane
- Nek5000 computational T/H